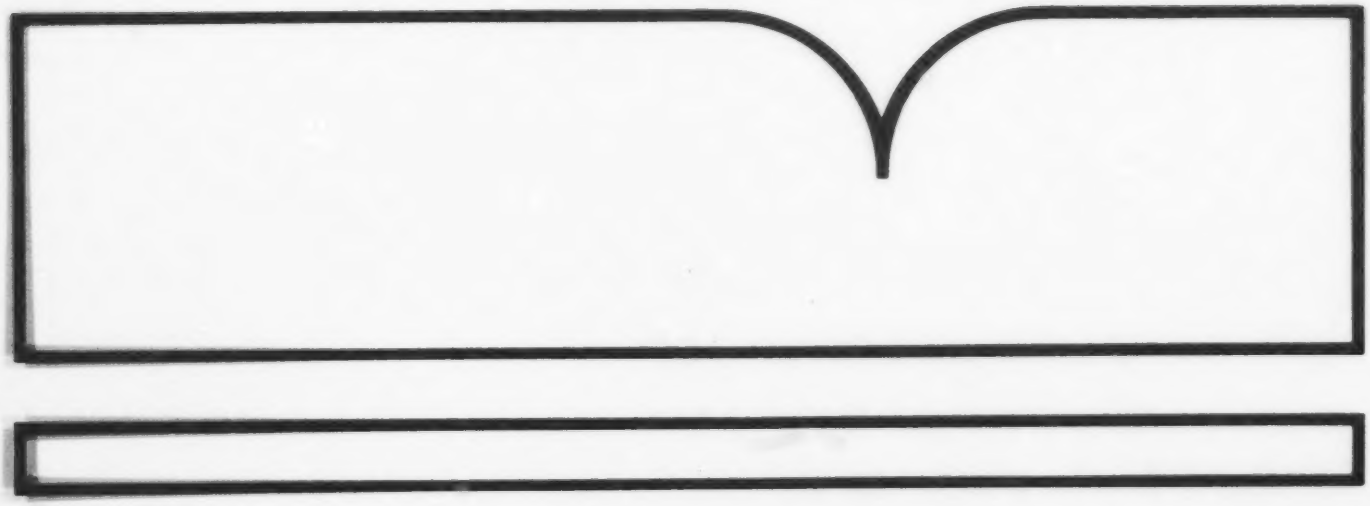
PB87-195400

Demonstration of INPUFF with the MATS Data Base

(U.S.) Environmental Protection Agency
Research Triangle Park, NC

1986



U.S. Department of Commerce
National Technical Information Service

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. PB87-195400
EPA/600/J-86/357		

4. TITLE AND SUBTITLE
A DEMONSTRATION OF INPUFF WITH THE MATS DATA BASE
(Journal Version)

5. REPORT DATE
1986

6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)
W. B. Petersen

8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Atmospheric Sciences Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

10. PROGRAM ELEMENT NO.
CDTA1D/04-1315 (FY-85)

11. CONTRACT/GRANT NO.

12. SPONSORING AGENCY NAME AND ADDRESS
Atmospheric Sciences Research Laboratory - RTP, NC
Office of Research and Development
U. S. Environmental Protection Agency
Research Triangle Park, NC 27711

13. TYPE OF REPORT AND PERIOD COVERED

14. SPONSORING AGENCY CODE
EPA/600/09

15. SUPPLEMENTARY NOTES
REF: Atmos. Environ., 20(7):1341-1346, July 1986

16. ABSTRACT

An integrated puff model, INPUFF, is evaluated using the MATS data base. A description of the model is provided outlining the salient characteristics. A brief description of the MATS data base, which consists of 14 SF_6 tracer releases with associated meteorology, is also provided. INPUFF slightly overestimated peak concentrations. Since the SF_6 puffs were well mixed for every tracer release, model performance is very sensitive to estimates of the mixing heights. The absolute mean fractional error between two techniques for estimating the mixing height was 0.87, which indicates a large uncertainty in this very important input parameter.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

REPRODUCED BY
U.S. DEPARTMENT OF COMMERCE
NATIONAL TECHNICAL
INFORMATION SERVICE
SPRINGFIELD, VA 22161

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS (This Report)	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	8
	20. SECURITY CLASS (This Page) UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

This article documents research that was conducted under the auspices of the U.S. Environmental Protection Agency (USEPA). As an arm of the government, the USEPA has a paid up, non-exclusive, irrevocable, worldwide license to reproduce, prepare derivative works, and distribute to the public all of the material contained herein, and to grant others acting on its behalf the right to do so. The USEPA grants to the National Technical Information Service, Department of Commerce, the right to act as its agent in the distribution of this material.

EPA/600/J-86/357
JOURNAL ARTICLE

Atmospheric Environment Vol. 20, No. 7, pp. 1341–1346, 1986.
Printed in Great Britain.

0004–6981/86 $3.00 + 0.00
Pergamon Journals Ltd.

A DEMONSTRATION OF INPUFF WITH THE MATS DATA BASE

WILLIAM B. PETERSEN*

Meteorology and Assessment Division, Atmospheric Sciences Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711, U.S.A.

(*First received* 28 *March* 1985 *and in final form* 8 *October* 1985)

Abstract—An integrated puff model, INPUFF, is evaluated using the MATS data base. A brief description of the model is provided outlining the salient characteristics. A description of the MATS data base, which consists of 14 SF_6 tracer releases with associated meteorology, is also provided. INPUFF slightly overestimated peak concentrations. Since the SF_6 puffs were well mixed for every tracer release, model performance is very sensitive to estimates of the mixing heights. The absolute mean fractional error between two techniques for estimating the mixing height is 0.87, which indicates a large uncertainty in this very important input parameter.

Key word index: Air quality model, model evaluation, puff model, tracer data base.

1. INTRODUCTION

During 1983 the Savannah River Laboratory (SRL) performed a tracer study consisting of 14 sulfur hexafluoride (SF_6) releases. Each release was 15 min in duration, and monitors were placed 20–30 km downwind. Sampling duration for the monitors ranged from 7 to 20 min, depending upon the experiment. Meteorological data, including turbulence measurements, were obtained at the 366-m WJBF TV tower (instrumented up to 306 m) and seven 61-m towers. Other meteorological data include the NWS upper air data from Charleston, South Carolina, and Athens, Georgia. These data are referred to as the Mesoscale Atmospheric Transport Studies (MATS) data base.

The MATS data were used to demonstrate the performance of INPUFF. INPUFF is a Gaussian integrated puff model. It is designed to simulate a semi-instantaneous or continuous point source release over a spatially and temporally varying wind field. Each of the 14 SF_6 releases was modelled with INPUFF. This paper presents a brief description of INPUFF, an overview of the MATS data, and the results of analysis of the performance of INPUFF with the MATS data.

2. DESCRIPTION OF INPUFF

There have been a number of puff and segmented plume models developed to simulate a broad range of modeling applications. In general, they are used where straight line Gaussian plume models do not apply. Models such as MESOPUFF II (Scire *et al.*, 1984) simulate regional transport where wind shear and non-homogeneity in terrain and meteorology present special modeling problems. Other puff models are designed to assess the air quality impact of toxic releases from a source of short duration (Palazzi *et al.*, 1982). Processes like negative buoyancy, gravity flow and temporally varying emissions present a different set of modeling problems. Hanna (1983) provided a survey of models developed for emergency response. This section will provide a brief description of INPUFF. A more complete description is available in the user's guide to INPUFF (Petersen *et al.*, 1984).

INPUFF is a Gaussian integrated puff model with a wide range of applications. The implied modeling scale is from tens of m to tens of km. The model is capable of addressing the accidental release of a substance over several minutes, or of modeling the more typical continuous plume from a stack. INPUFF is also capable of simulating a moving point source. Three dispersion algorithms are available within INPUFF for characterizing the dispersion downwind of the source. The user may choose the Pasquill–Gifford (P–G) scheme (Turner, 1970) or the on-site scheme (Irwin, 1983) for short travel times. The on-site scheme, so named because it requires specification of the standard deviations of the vertical and lateral wind directions, is a synthesis of the work performed by Draxler (1976) and Cramer (1976). The third dispersion scheme is for long travel times in which the growth of the puff becomes proportional to the square root of time.

The dispersion curves of the P–G scheme mentioned above are well documented. In view of this, only a summary of the on-site scheme is presented. This scheme is consistent with the recommendations of the American Meteorological Society's workshop on stability classification schemes and sigma curves (Hanna *et al.*, 1977). Irwin (1983) proposed characterizing σ_y and σ_z in a manner similar to Cramer (1976) and Draxler

*On Assignment from the National Oceanic and Atmospheric Administration, Dept. of Commerce.

(1976). The standard deviation of the crosswind concentration distribution, σ_y, is

$$\sigma_y = \sigma_v t f_y$$

where σ_v is the standard deviation of the lateral component of the wind, t is the travel time of the pollutant, and f_y is a nondimensional function of travel time. The standard deviation of the vertical concentration distribution, σ_z, for an elevated source, when σ_z is less than the source height, is

$$\sigma_z = \sigma_w t f_z$$

where σ_w is the standard deviation of the vertical component of the wind, and f_z is a nondimensional function, primarily dependent upon travel time. The nondimensional functions f_y and f_z were characterized by Irwin (1983) as

$$f_y = 1/[1 + 0.9(t/1000)^{1/2}] \quad \text{for all stabilities}$$

$$f_z = \begin{cases} 1, & \text{for unstable conditions} \\ 1/[1 + 0.9(t/50)^{1/2}], & \text{for stable conditions.} \end{cases}$$

The puff model requires σ_a and σ_e as data input to use the on-site scheme. For small angles, $\sigma_v = \sigma_a u$ and $\sigma_w = \sigma_e u$, where u is the wind speed at measurement height and σ_a and σ_e are the standard deviations of the horizontal and vertical wind angles, respectively. The Pasquill and on-site dispersion schemes are applicable for plume dispersion where the sampling time is much greater than the travel time from the release point to the receptor. For the MATS data, travel times were greater than the sampling time and puff dispersion should apply. Although plume sigmas should theoretically overpredict horizontal diffusion, Allwine and Whitemar (1985) deduce that empirical plume dispersion coefficients may not be a bad estimate of puff dispersion for longer travel times. A typical value of σ_y (puff dispersion) for travel times of 1–3 h is 2000 m (Hanna *et al.*, 1982). By comparison, σ_y values were computed using the travel times and average values given in Table 3. Estimates of σ_y ranged from a minimum of 1298 m to a maximum of 3268 m with an average value of 1693 m. This suggests that the plume dispersion parameters used in INPUFF are not unreasonable for this application.

3. INPUT DATA

The MATS data base consists of meteorological data, as well as SF_6 emissions and measurements. The meteorological data include 15-min averages of wind direction and speed, standard deviations of wind azimuth and elevation angle, and temperature. Data were measured on seven 61-m towers and at seven levels on the 366 m WJBF TV tower (18, 36, 91, 177, 182, 243 and 304 m). The UTM coordinates of the meteorological towers and the 91-m stack where the SF_6 was released are given in Table 1. A site map of the Savannah River Plant is shown in Fig. 1. Estimates of the maximum mixing heights during the 14 tracer releases were determined using the upper air soundings from Athens. Mixing heights were also estimated using the Charleston data, but it was felt that the ocean environment unduly influenced the height of the mixed depth layer. Estimates of the maximum mixing heights were also provided by SRL, using Garrett's model (1981), and are listed in Table 2.

Table 1. UTM coordinates of meteorological towers and SF_6 release site

Met. towers	Height (m)	North (km)	East (km)
WJBF tower	366	3696.308	422.146
A	61	3688.754	431.264
C	61	3679.014	437.017
D1	18	3673.972	431.270
D2	61	3673.972	431.270
F	61	3683.073	437.095
H	61	3683.338	440.046
K	61	3674.695	438.181
P	61	3676.528	445.957
SF_6 release site	91	3683.592	439 199

The SF_6 tracer was vented through a 91-m stack. Stack effluents were at ambient temperature with a stack gas exit velocity of 6.6 m s^{-1}. Sequential samplers provided from 7 to 20 min average SF_6 concentrations, depending on the particular experiment. The sampling array provided concentrations at approximately 1 km spacing along an arc from 20 to 30 km downwind, depending on the particular experiment. Table 3 shows the experiment number, date and time of release, SF_6 emission rate, number of samplers, and the sampling interval.

4. MODEL COMPARISONS

The meteorological data described above were used as input into INPUFF. For these simulations the winds were assumed to be homogeneous in space. Therefore, for each 15-min period a single value of wind transport and diffusion were input into the model. Wind direction, speed, and turbulence parameters input into the model were computed from the

Table 2. Estimates of maximum mixing heights (m)

Experiment No.	Charleston	Athens	Garrett
1	301	332	800
4	140	557	1849
5	1908	582	1922
7	1011	1146	2738
8	1909	1529	2178
9	1785	1220	2592
12	1776	1063	1682
13	1600	1066	1800
14	896	1108	882
15	570	913	648
16	1016	1427	968
17	1273	922	1152
18	Missing	1642	1352
19	480	603	1058

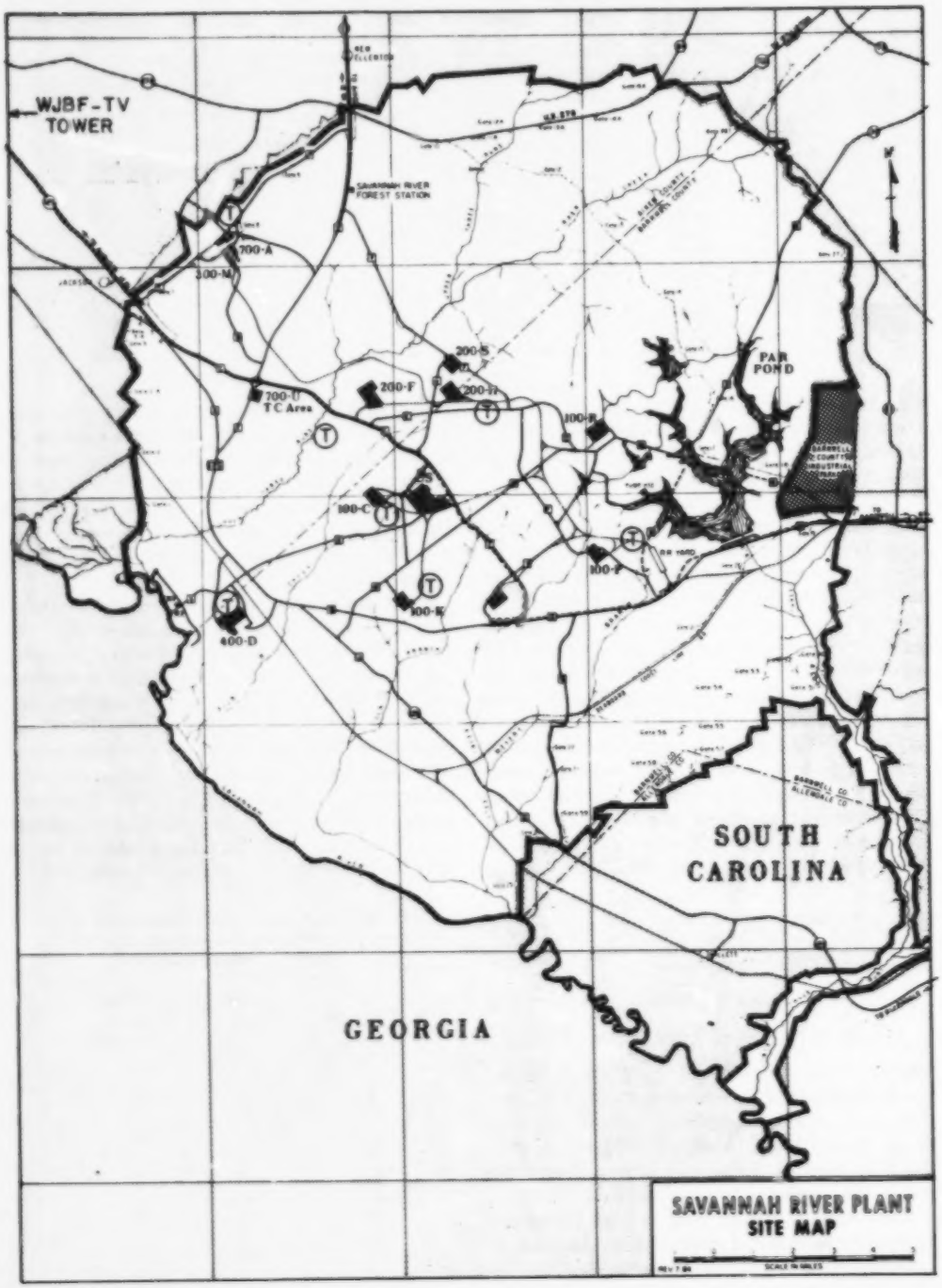


Fig. 1. Savannah River plant site map. The circled Ts indicate locations of meteorological towers.

Table 3. Aerometric data for the 14 SF_6 releases

Exp. No.	Date	Time of release (GMT)	SF emission rate ($g\,s^{-1}$)	Number of samplers	Sampling interval (min)	Wind speed ($m\,s^{-1}$)	Wind direction (deg)	Std. deviation wind direction (deg)
1	27-1-83	16:15	35.07	16	5	6.4	46	8.7
4	20-5-83	15:15	19.7	19	7	5.2	208	10.0
5	1-6-83	16:30	40.6	18	10	6.5	332	9.3
7	7-7-83	14:35	78.3	19	10	3.3	39	28.2
8	22-7-83	14:30	63.33	18	15	3.7	260	13.5
9	29-7-83	15:45	66.11	17	15	5.4	69	16.4
12	28-9-83	14:30	88.9	19	15	5.5	27	11.6
13	7-10-83	14:30	27.8	19	15	6.7	67	11.9
14	17-10-83	14:00	110.5	19	15	3.4	75	8.9
15	21-10-83	13:45	101.0	19	15	5.7	34	8.7
16	2-12-83	15:45	65.6	29	20	2.9	175	15.6
17	9-12-83	15:15	56.1	30	15	3.5	160	16.1
18	15-12-83	15:45	91.6	30	20	4.5	265	12.1
19	20-12-83	16:00	80.0	27	16	5.1	27	11.7

three meteorological towers nearest the release point. The mean of each parameter was computed and then adjusted to release height by using the profiles of meteorological data on the WJBF TV tower. Because of its distance from the release point the WJBF tower was never one of the near three towers used in the computation of the mean values. For a given experiment, the model was executed and compared with observations. A single wind direction correction was computed that transported the SF_6 through the monitoring array at approximately the same location as the observations. The wind direction adjustment was applied to each 15-min wind direction used in the simulation, and the model was rerun with the adjusted winds. The wind direction correction was never greater than 7 degrees. The minimum and maximum mixed depth layer for each experiment were computed from the temperature soundings from Athens, Georgia. Estimates of the height of the mixed layer for each 15-min period were computed from the following formulas:

$$Z_i' = Z_m(-0.02 + 0.25\,T^* + 3.30\,T^{*2}) \quad \text{for } T^* < 0.52$$

$$T^* = (T_L - SR)/(SS - SR)$$

$$Z_i' = Z_m(0.119 + 3.26\,T^* - 3T^{*2}) \quad \text{for } T^* > 0.52$$

$$Z_i = \text{MAX of } (Z_i' \text{ and the minimum mixing height})$$

where Z_m is the maximum mixing height, T_L is the local standard time, SR is the time of sunrise, and SS is the time of sunset. The above equations are empirical fits to the diurnal variation of mixing heights at rural locations from St. Louis and Zagreb, Yugoslavia (Irwin, 1984, personal communication).

The aerometric data provided in Table 3 were used as input for INPUFF. A comparison of the transport time predicted by the model and that inferred from the observations showed significant differences. For example, in Experiment 8 the model predicted that the SF_6 would arrive 1 h later than it actually arrived. Because of this, the wind speeds were recomputed using the layer-averaged wind speed from all levels on the WJBF tower. INPUFF was again executed using these layer-averaged wind speeds. The differences between the inferred transport times and the estimated times are presented in Table 4. A zero indicates that the model estimated a transport time the same as that inferred from observations. In general the layer-averaged winds provided a slightly better characterization of the transport speed.

Using the layer-averaged wind speeds, the estimated peak concentrations for each experiment were compared with observed peak concentrations. A scatter plot of peak concentrations normalized by emission rate is shown in Fig. 2. The one-to-one line (solid line) is displayed for reference with the regression fit shown as the dashed line. The correlation coefficient is 0.54. The peak dosages normalized by mass for each experiment are plotted in Fig. 3. The correlation coefficient is 0.30. However, it is significantly improved to 0.59 when the results from Experiment 18 are not included in the regression analysis. The data point in

Table 4. Differences in transport time between model estimates and those inferred from SF_6 observations (min)

Exp. No.	Profile winds	Layer averaged winds
1	0	0
4	21	0
5	30	60
7	30	−10
8	60	60
9	0	0
12	0	0
13	−15	0
14	−15	−75
15	0	0
16	20	0
17	0	−15
18	0	0
19	0	32

A positive value indicates the SF_6 arrived later than anticipated from the observations.

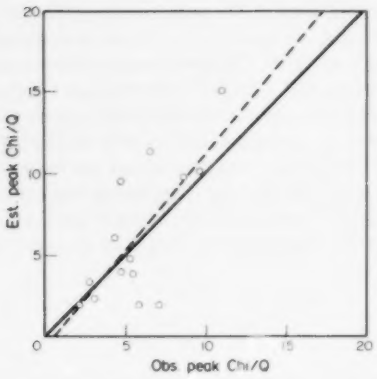


Fig. 2. Estimated normalized peak concentration vs observed normalized peak concentration.

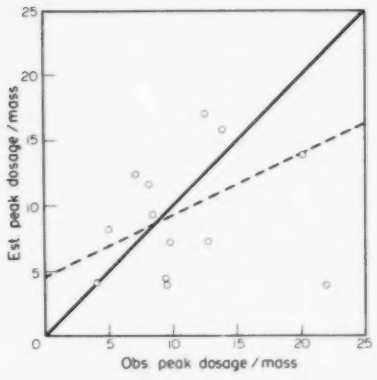


Fig. 3. Estimated normalized peak dosage vs observed normalized peak dosage.

the lower righthand corner is from Experiment 18. The dosages at all monitors for Experiment 18 are greatly underestimated by the model. The peak normalized concentration is also underestimated by about a factor of three. Our first thought was that the mixing height had been greatly overestimated. However, a review of the estimates of Z_m from Table 2 does not suggest this is the case, since there is good agreement between an analysis of the temperature data at Athens and the estimates of Z_m using Garrett's method. A factor of two difference in dispersion rates from those used in the model and those that actually dispersed the puff would account for the large difference. However, two other possible causes are a locally shallow mixing height at the release site or an incorrect emission rate. The mean fractional error (twice the difference of estimated minus observed divided by the sum of estimated plus observed) of the peak normalized concentrations and dosages are -0.06 and -0.18, respectively. If the results from Experiment 18 are omitted, then these values are 0.02 and -0.08, indicating a slight tendency for the model to overpredict peak concentrations and a slight tendency to underestimate dosages.

The above analyses indicate a large amount of scatter in the model estimates. Even more scatter would be anticipated with the model estimates for each monitor for each sampling period. Therefore, it was decided to analyze the data using a different approach. During all of the experimental releases the SF_6 was well-mixed by the time it reached the monitoring array. For a well-mixed puff, assuming streamwise and crosswind dispersion are equal, the peak concentration is given by

$$C_p = Q/(2\pi\sigma_y^2 L)$$

where C_p is the peak concentration, Q is the total mass released, σ_y is the lateral dispersion coefficient, and L is the height of the mixed depth layer. The above equation can be rearranged and rewritten in the following form

$$(C_p L/Q)^{1/2}\,\sigma_a U = 1/(\sqrt{2\pi}\, f_y t)$$
$$f_y = 1/(1+0.9\,(t/1000)^{1/2}) \qquad (1)$$

where σ_a is the standard deviation of the azimuth angle, U is the wind speed, and t is the travel time. The solid lines in Figs 4a and 4b are the equation $1/(\sqrt{2\pi}\, f_y t)$. The peak observed concentrations are used in Equation (1) and plotted in Fig. 4a. Modeled peak concentrations are plotted in Fig. 4b for different travel times. One would certainly expect a better fit to the theoretical curve with the model estimates than the observations, and in fact this is so. The results from Experiments 1 and 8 are further off the theoretical curve than the other experiments, but, in general, the model follows the theoretical curve. Several factors contribute to model estimates not falling exactly along the theoretical curve. Average σ_a and U values were used in Equation (1), whereas unique σ_a and U values for each sampling period were used in the model estimates. The peak concentration estimate probably did not occur exactly at one of the monitoring sites. Since concentration estimates were performed only at the monitoring sites, the value of Equation (1) may not fall along the theoretical curve. The observed peak concentrations, plotted in Fig. 4a, show considerable scatter, although the theoretical trend is in the data. Four of the experiments produced data above the curve and nine experiments produced results below the curve. Experiments 1, 4, 7, 8, 14 and 18 produced results that are particularly far from the curve, especially Experiments 1 and 7.

Uncertainties in the parameters mentioned above and the possibility of physical processes occurring that are not being addressed in the model account for the scatter in the observations. The results from Wilczak and Phillips (1984) suggest that even with state of the art instrumentation the uncertainty in the estimates of

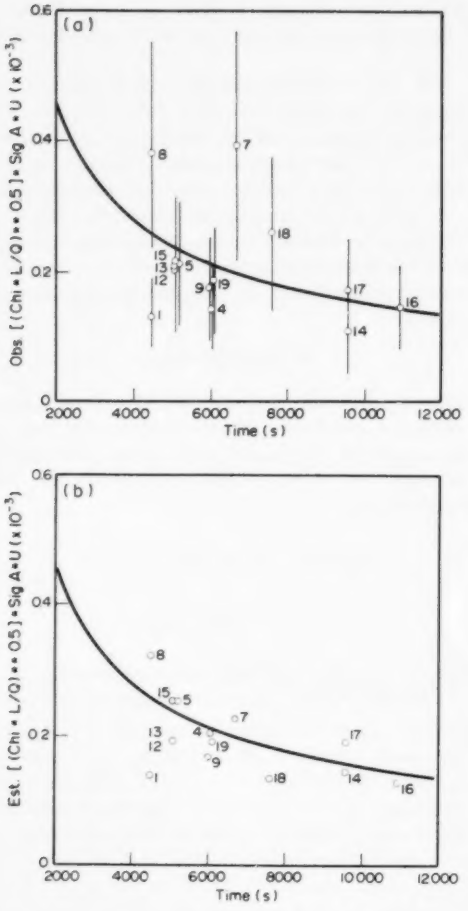


Fig. 4. (a) Observed peak concentrations vs transport time. (b) Estimated peak concentrations vs transport time.

the mixing height is 30%, and the uncertainty in the wind speed and fluctuation statistics is between 10 and 30%. For illustration purposes an uncertainty of 30% was assumed for L and an uncertainty of 15% assumed for U and σ_a. The gross error introduced in Equation (1) is then $\pm 45\%$. The whisker lines in Fig. 4a are the observed values $\pm 45\%$. In 11 of the 14 experiments the uncertainty in L, U and σ_a suggests that the observations are consistent with the theory.

5. CONCLUSIONS

Model estimates of SF_6 concentrations were compared with observations. Figure 2 suggests that INPUFF slightly overestimates highest peak concentrations and has a slight bias towards underprediction of the peak dosage. The large amount of scatter in the model estimates may be due to the large uncertainty in the mixing heights. The absolute mean fractional error between the mixing heights inferred from temperature soundings and those estimated from Garrett's model is 0.87 with a standard deviation of 0.74. During well-mixed conditions concentrations are inversely proportional to the mixing height, suggesting that a meaningful model evaluation exercise would require a more precise specification of the height of the mixed depth layer.

REFERENCES

Allwine K. J. and Whitemar C. D. (1985) Green river air quality model development melsar—a mesoscale air quality model for complex terrain. EPA-600/8-85/017a, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Cramer H. E. (1976) Improved techniques for modeling the dispersion of tall stack plume. In *Proceedings of the Seventh International Technical Meeting on Air Pollution Modeling and its Application*. No. 51, NATO/CCMS, pp. 731–780 (NTIS PB 270 799).

Draxler R. R. (1976) Determination of atmospheric diffusion parameters. *Atmospheric Environment* **10**, 99–105.

Garrett A. J. (1981) Comparison of observed mixed-layer depths to model estimates using observed temperatures and winds, and MOS forecasts. *J. appl. Met.* **11**, 1277–1283.

Hanna S. R. (1983) A survey of emergency models and applications—I. Models developed for hazardous spills applications. In *The 76th Annual Meeting of the Air Pollution Control Association*, Atlanta, Georgia, 83-26.1.

Hanna S. R., Briggs G. A., Deardorff J., Egan B. A., Gifford F. A. and Pasquill F. (1977) AMS-workshop on stability classification schemes and sigma curves—summary of recommendations. *Bull. Am. met. Soc.* **58**, 1305–1309.

Hanna S. R., Briggs G. A. and Hosker R. P., Jr. (1982) *Handbook on Atmospheric Diffusion*, DOE/TIC-11223, U.S. Department of Energy, Technical Information Center, Oak Ridge, TN.

Irwin J. S. (1983) Estimating plume dispersion—a comparison of several sigma schemes. *J. Clim. appl. Met.* **22**, 92–114.

Palazzi E., De Faveri M., Fumarola G. and Ferraiolo G. (1982) Diffusion from a steady source of short duration. *Atmospheric Environment* **16**, 2785–2790.

Pasquill F. (1961) The estimation of the dispersion of windborne material. *Met. Magazine* **90**, 33–49.

Petersen W. B., Catalano J. A., Chico T. and Yuen T. S. (1984) INPUFF—a single source Gaussian puff dispersion model user's guide. EPA-600/8-84-027, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Scire J. S., Lurmann F. W., Bass A. and Hanna S. R. (1984) User's guide to the MESOPUFF II model and related processor programs. EPA-600/8-84-013, U.S. Environmental Protection Agency, Research Triangle Park, NC (NTIS PB 84-181 755).

Turner D. B. (1970) Workbook of atmospheric dispersion estimates. Office of air programs publication No. AP-26 (NTIS PB 191 482). U.S. Environmental Protection Agency, Research Triangle Park, NC.

Wilczak J. M. and Phillips M. S. (1984) An indirect estimation of convective boundary layer structure for use in routine dispersion models. *Proceedings of the Fourth Joint Conference on Applications of Air Pollution Meteorology*, Portland, Oregon, pp. 16–19.